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Mathematical Software Overview

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Preface

Scope: This Mathematical Software Overview introduces the approach to math software taken at LC, compares the chief math subroutine libraries available, and explains the lookup and support tools (including reference manuals) that help you use those libraries effectively. It also introduces a few important, commercial, interactive math tools available at LC (Mathematica, MATLAB, and Tecplot).

Availability: Not all math tools and libraries are available on all machines. Also, you must decide between compiled and installed math libraries that offer convenience but perhaps narrow technical choices or source-code packages from LINMath that offer greater flexibity but demand more customization from you. See the more thorough discussion of availability issues for math libraries in the dedicated section (page 5) below.

Consultant: For help contact the LC customer service and support hotline at 925-422-4531 (open e-mail: lc-hotline@llnl.gov, secure e-mail: lc-hotline@pop.llnl.gov).

Printing: The print file for this document can be found at

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OCF: https://computing.llnl.gov/LCdocs/math/math.pdf
SCF: http://www.llnl.gov/LCdocs/math/math_scf.pdf
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Introduction

The belief behind LC's approach to mathematical software support is that computational tasks required in a wide variety of applications share common, mathematically defined features, to which general purpose techniques can be applied. This results in a long-term overall cost savings, through software reuse and reduced duplication of effort.

This approach was long embodied in LC's very fruitful Mathematical Software Service (MSS, see the next section). It is still reflected in the surviving products of that former group, including local libraries (such as PMATH) and local math self-help tools for numerical mathematics (such as the LINMath (page 11) Web site). This document surveys those libraries and tools, compares their features, and offers links to the current reference documentation for each one.

Former MSS Group

Formerly, the focus of math support at LC was a separate Mathematical Software Support Service (MSS). Although the MSS has disbanded, its many useful products remain in play (and their sources are user-movable to new platforms). The former MSS consulting duties now fall to the central LC Hotline staff, and this introductory document replaces the former MSS home page as the online focal point for basic math-support information.

Math Libraries Chart

Users often ask which mathematics libraries are "available" on which LC systems. The answer depends on what you regard as availability, and on how much customization you need (or are willing to perform).

Preinstalled.
On each LC operating system (AIX and Linux/CHAOS) some math libraries, mostly from commercial vendors, are preinstalled as compiled (object) code. Even here there are decisions to be made. The libraries sometimes overlap (several versions of BLAS are installed on AIX, for example). Some routines are optimized for the operating system where they reside and some are not; some are threaded and some are not; some are portable and some are not; some are single or double precision. Only your own computational needs can clarify which of these competing libraries are most appropriate for your work.

Downloadable.
Beyond the relatively small set of compiled, preinstalled math libraries (around a dozen) is a much larger set of downloadable source-code math-routine "packages" (around 140 for OCF systems, 13 on SCF). These often specialized or customizable packages are not proprietary and most are widely shared among the research community of computational mathematicians. At LC, the LINMath (page 11) Web site describes, compares, and (if you wish) actually distributes the source code for these extra math packages (as well as the sources for isolated math routines). Again, these collaborative packages often overlap each other and the commercial libraries (and again, BLAS illustrates that overlap). So you must decide which alternatives best meet your current, specific needs.

Availability Chart.
This chart provides a very short, simplified answer to the math-library availability question. It shows at a glance which major libraries reside on which LC machines. But for the richer, more complex answer suggested above, you need to consult the "AIX Libraries" section (page 7) as well as the "LINMath" section (page 11) below for useful, comparative technical detail.

	Platform/OS	
	IBM/AIX	Intel/Linux
Installed as compiled (object) code	LIBM(*)	PMATH
	ESSL	
	PESSL	MKL
	FFTW (OCF)	FFTW (OCF)
	SPRNG	SPRNG
	LAPACK	
	PARMETIS	
Downloadable from LINMath (you compile)	PMATH	PMATH
	SLATEC	SLATEC
	MSSL	MSSL

[NOTE: PMATH, SLATEC, and MSSL are all available from the LINMath (page 11) Web site as source code, which you can then move to any machine and compile.]

(*)Beginning in May 2003, LC provides preinstalled on all IBM/AIX machines (open and secure) the Mathematical Acceleration Subsystem (MASS, or libmass.a), which offers "tuned alternatives" for many LIBM functions to help optimize codes. Vendor support is available at the (open only) Web site:

http://techsupport.services.ibm.com/server/mass?fetch=home.html

Math library users may also want to be aware of ZLIB (libz.a), a lossless, general-purpose data-compression (and decompression) library available for many computer platforms and operating systems (its compression algorithm is the same as that used for the ZIP and UNZIP tools). ZLIB (libz.a) is preinstalled (with support for both 32- and 64-bit executables) on LC Linux/CHAOS and AIX machines in /usr/lib (replaces a former, outdated version once in /usr/local/lib). See also

http://www.zlib.net

AIX Math Libraries

Below are the compiled, preinstalled mathematics libraries available on LC's AIX (IBM) machines, with comparative usage advice on each. For more background on library "availability" issues, see the previous section (page 5).

LIBM
/usr/lib/libm.a

is the standard C math library from IBM (see also MASS, below).

MASS
/usr/lib/libmass.a

is the Math Acceleration SubSystem from IBM. This includes high performance versions of many of the double-precision routines from LIBM (above). Results may differ by a few units in the last place.

MASSV
/usr/lib/libmassv.a
/usr/lib/libmassvp2.a
/usr/lib/libmassvp3.a
/usr/lib/libmassvp4.a
/usr/lib/libmassvp5.a

contains optimized single- and double-precision vector versions of routines from MASS (above), plus some additional math intrinsics. Results may differ from LIBM, MASS, and compiler-generated code by a few units in the last place. Multiple versions of MASSV are optimized for Power5, Power4, and Power3 IBM chips (see pathnames at left).

BLAS
/usr/lib/libblas.a

includes all the original Level-1, Level-2 and Level-3 BLAS routines (Basic Linear Algebra Subroutines) except DSDOT. We don't know if these routines are really optimized for AIX machines, but we recommend that you use ESSL (below) instead. If you need the handful of routines in BLAS that are not in ESSL, link BLAS *after* ESSL so that ESSL's optimized routines are resolved first:
... -lessl -lblas

ESSL
/usr/lib/libessl.a

is IBM's Engineering Scientific Subroutine Library. ESSL provides a variey of optimized complex mathematical functions for many different scientific and engineering applications such as Basic Linear Algebra Subroutines (BLAS), linear algebraic equation solvers and eigensystem analysis (a subset of LAPACK), Fast Fourier Transforms (FFTs), sorting, searching, quadrature, and random number generation. ESSL provides single- and double-precision versions for most routines.

ESSL includes all the BLAS that come with the LAPACK distribution (below). But it does not include the following original BLAS routines, most of which are in libblas.a: CSROT, DROTM, DROTMG, DSDOT, SDSDOT, SROTM, SROTMG, ZDROT.

Some ESSL eigenvalue routines have the same name as LAPACK routines (see below) but are different (since ESSL predates LAPACK). If you want to use the LAPACK routines whose names conflict with routines in ESSL, use the AR tool to split ESSL into two libraries: one with just the conflicting routines, say, libconflict.a, and the other with the rest of the routines, say, libesslnoconflict.a. Link the noconflict routines *before* the full LAPACK library:
... -lesslnoconflict -llapack
This gives you optimized versions of the LAPACK routines that are in ESSL, with liblapack.a resolving all the other routines.

ESSL.SMP
/usr/lib/libesslsmp.a

is the threaded version of ESSL. Many routines here have been parallelized for shared memory nodes.

PESSL
/usr/lib/libpessl.a
/usr/lib/libpesslsmp.a
/usr/lib/libblacs.a
/usr/lib/libblacssmp.a

is IBM's Parallel Engineering Scientific Subroutine Library. PESSL is a parallel version of the ESSL library (above). It is used in conjunction with the serial version of ESSL. It contains a number of Parallel BLAS (PBLAS), Basic Linear Algebra Communication Subprograms (PBLACS), and ScaLAPACK routines.

LAPACK
/usr/local/lib/liblapack.a

is a comprehensive, well-respected, and freely distributed library of software for linear algebra. It is based on the Level-2 and Level-3 BLAS and should be used in conjunction with a vendor-supplied optimized BLAS library (such as ESSL, see above). LAPACK provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems.

FFTW
/usr/local/lib/libfftw.a
/usr/local/lib/libdfftw.a
/usr/local/lib/libdrfftw.a
/usr/local/lib/librfftw.a
/usr/local/lib/libsfftw.a

/usr/local/lib/libsrfftw.a

is a nonproprietary C library for computing Discrete Fourier Transforms. See its own section (page 20) below.

PMATH
/usr/lib/libpmath.a

is a portable version of the former MATHLIB library. See its own section (page 18) below.

PARMETIS
/usr/lib/libparmetis.a

is the Parallel Graph Partitioning and Sparse Matrix Ordering Library. This is an MPI-based parallel library that partitions unstructured graphs and meshes, and that computes fill-reducing orderings of sparse matrices.

MATHEMATICA

is an interactive package for symbolic computation and complex analysis. See its own section (page 24) below.

NMG (Retired)

NMG (the "numerical mathematics guide") was an interactive utility that provided guidance for and access to the LC-supported math libraries. NMG helped users select appropriate math subroutines for specified computational tasks, and then let them retrieve documentation or (when nonproprietary) source code for the subroutines selected.

NMG retired from public service along with LC's secure CRAY J90 computers in March 2000. However, most NMG functions live on in a different form as various levels in the LINMath (page 11) Web site, described in the next section.

LINMath Web Site (Tool)

LINMath (Livermore Interactive Numerical Mathematics software access utility) is a customized Web site that delivers advice on and descriptions of mathematical library subroutines, as well as the subroutine source files themselves. The LINMath Web site uses the standard GAMS (URL: https://computing.llnl.gov/LCdocs/gams) (Guide to Available Mathematical Software) hierarchical system for organizing math routines to structure its menu tree.

The LINMath Web site offers most of the same math-help functions formerly provided by the now-defunct CRAY NMG utility, only in a different way (as hypertext). Also, LINMath provides the most recent, debugged versions of SLATEC and PMATH routines (*more* recent than the versions installed on some LC machines as compiled object code).

LINMath Features

To use the LINMath Web site, execute any standard WWW browser (client) and request the open URL

`http://www-lc.llnl.gov/linmath/`

As the URL implies (www-lc), the LINMath server automatically restricts access to only those clients running on machines within the LLNL domain(s). A comparable LINMath site is available within the LLNL secure network at the SCF URL

`http://www.llnl.gov/linmath`

Users of the former NMG tool will recognize LINMath as a Web-based version of NMG. Of course, LINMath relies on interactive hypertext links and other common Web browser (client) features, rather than on commands typed in response to prompts, to navigate its structure and ultimately to deliver appropriate mathematical software. Partly for this reason, LINMath combines into a single menu tree the advice, menu, and fetch (download) features that were once available as separate NMG commands. LINMath covers the most up-to-date versions of the SLATEC, MSSL, and PMATH subroutine libraries directly, with indirect support for other, external math libraries.

LINMath Documentation

LINMath's basic instructions, access restrictions, and practical usage tips are all covered in the LINMath User Guide (URL: https://computing.llnl.gov/LCdocs/nmg1). This manual also compares the top, middle, and bottom levels of the LINMath tree with the menu, advice, and fetch commands of the former NMG utility, respectively.

Because the LINMath site is divided among many separate files, you cannot display (or print) the entire GAMS classification scheme from the site itself. If a comprehensive and comparative overview of the entire GAMS scheme would help you with LINMath planning and subroutine decisions, consult the separate GAMS online document (URL: https://computing.llnl.gov/LCdocs/gams). This document contains NIST's complete Guide to Available Mathematical Software.

You can easily display or print (with File/Print) the full set of subject headings for any GAMS subject category using your WWW client. Or you can print the entire 36-page GAMS document for reference by getting its PDF file from either the open or secure LC documentation server and using the printing directions and link offered in the first section (preface) of the GAMS Guide itself.

LINMath Packages

Because of their unusual usefulness, some nonproprietary packages of math subroutines receive featured support from LINMath. On both OCF and SCF, the LINMath main (home) page offers a link to an alphabetized list of supported math packages (about 140 on OCF, only 13 on SCF). Pursuing any name in the package list yields descriptive background information (arranged by GAMS category) and then direct download access to the subroutine source code (for authorized users, so access may vary by user and by package).

Because the LINMath site text is not searchable the way this manual is, we reprint here the alphabetical list of mathematical subroutine packages for which LINMath provides this featured support (all are OCF, those explicitly marked are also SCF). You may want to compare these source-code sets with libraries already compiled and installed on your target machine to determine which alternatives best meet your specific computational needs (for example, see the "AIX Libraries" section (page 7) above).

```
A
AMOS [SCF also]
AMPL
ARPACK
AZTEC
BERKELEY-LAB-AMR
BIHAR
BLACS
BLAS [SCF also]
BLOCKSOLVE95
BMP
BPKIT
BPMPD
BRENT [SCF also]
CACTUS
CEPHES
CLAPACK
CONFORMAL
CVODES
DAEPACK(MIT)(Nonlinear eqns)
DAEPACK(MIT)(ODEs/DAEs)
DAEPACK(MIT)(Symbolic comp)
DAEPAK(U.Pitt.)
DEAL
DIERCKX
DIFFPACK
DOUG
EISPACK-S [SCF also]
EISPACK-D
ELEFUNT
FDLIBM
FFTPACK
FFTW
FIDISOL/CADSOL
FISHPACK [SCF also]
FITPACK
FN
FORTRAN-M
GCV
GISOLV
GPS
GRAL
```

GRAPHICS
HSL(HARWELL)
HOMPACK
HYPRE
IDA
IMAGE
IML++
ITPACK
JAKEF
KELP
KINSOL
KNITRO
LANCZOS
LANZ
LAPACK
LASO
LASPACK
LAWSON-HANSON
LC-GRAPHICS [SCF also]
LINAL
LINALG
LINPACK [SCF also]
LSA(Linear-Systems-Analyzer)
LSODE [SCF also]
MANPAK
MDS
MEBDF
MESCHACH
METIS
MINPACK(Nonlinear-equations)
MINPACK(Optimization)
MODULEF
MOSEK
MPFUN
MTL
MUDPACK
NAPACK(Linear-equations)
NAPACK(Optimization)
NEOS
NETSOLVE
NLR
ODE
ODEPACK [SCF also]
ODEPACK(Collection)
ODRPACK
OPT
OPTIMIZATION-GUIDE
OVERTURE
PARANOIA
PARASAILS
PARASOL
PARPRE
PBLAS
PCHIP [SCF also]
PDES
PETSC
PLAPACK
PLTMG
PMLP
POOMA

PORT-LIBRARY
PPPACK
PSEUDOPACK(Differentiation)
PSEUDOPACK(FFT)
PSIDE
PSPARSLIB
PSPASES
QUADPACK [SCF also]
RANDOM
RK-CODES
SAMRAI
SBMETHOD(Linear-Algebra)
SBMETHOD(Optimization)
SCALAPACK
SLAP [SCF also]
SLDRIVER
SLICOT
SMINPACK(Nonlinear-equations)
SMINPACK(Optimization)
SOFTWARE-SURVEY
SPAI
SPARSE
SPARSE-BLAS
SPARSKIT
SPECFUN
S+
SPRNG
STOEPLITZ
SUPERLU
SVDPACK
TEMPLATES
TOEPLITZ
TRANSFORM
TRON
UMFPACK
VANHUFFEL
VFFTPACK
VFNLIB
VODPK [SCF also]
WSMP
Y12M

Math Libraries

This section introduces the NONPROPRIETARY math subroutine libraries that LC provides and (passively) supports.

SLATEC Library

Background

SLATEC is an acronym for the Sandia, Los Alamos, Air Force Weapons Laboratory Technical Exchange Committee. Formed in 1974 to foster exchange among these three New Mexico laboratories, it has since been expanded to include LLNL (both LC and the former NERSC), ORNL, and NIST (the National Institute for Standards and Technology, formerly NBS). On occasion, ANL, NCAR, and other Government laboratories have also been involved in SLATEC activities.

The Common Mathematical Library (CML) developed by SLATEC is a portable Fortran 77 library of high-quality mathematical software. It includes the widely-known packages BSPLINE, EISPACK, FISHPACK, FNLIB, LINPACK, PCHIP, QUADPACK and much more. (It is very weak in statistical software.)

Routines from this library, being nonproprietary and portable, may be used on both the LC mainframes and the user's workstation. SLATEC is neither installed nor supported on LC machines, but you can move source code that you get from LINMath. In fact, since the LINMath sources are more recent and more thoroughly debugged than the installed binaries, Linux users are also encouraged to prefer the LINMath version of all SLATEC routines.

Documentation

For those who use the SLATEC library, LC provides five supporting manuals:

SLATEC1 — provides introductory information on the whole SLATEC library, including background on five of the software "packages" it contains, descriptions of the SLATEC error procedure, and advice for interpreting SLATEC's highly stylized explanatory prologues. SLATEC1 introduces the GAMS subject categories (URL: https://computing.llnl.gov/LCdocs/gams) into which the SLATEC routines are grouped, and includes short descriptions of all routines (alphabetical within each subject category). Every category code is also a link (keyword) for retrieving the brief descriptions of the included routines, and every routine name links back to its category. SLATEC1 (with links) provides the only way to compare related routines by the tasks they perform, rather than just by name.

SLATEC2 — contains the calling sequence and usage details for each of the 225 subroutines from AAAAAA through D9UPAK, arranged alphabetically by name. Every subroutine name is also a link (keyword) for retrieving the corresponding description if you start at the index.

SLATEC3 — contains the calling sequence and usage details for each of the 225 subroutines from DACOSH through DS2Y, arranged alphabetically by name. Every subroutine name is also a link (keyword) for retrieving the corresponding description if you start at the index.

SLATEC4 contains the calling sequence and usage details for each of the 226 subroutines from DSBMV through RD, arranged alphabetically by name. Every subroutine name is also a link (keyword) for retrieving the corresponding description if you start at the index. (NOTE: At LC, use service routines I1MACH and R1MACH (page 29) from MSSL (page 19) rather than from SLATEC for more accurate results.)

SLATEC5 contains the calling sequence and usage details for each of the 226 subroutines from REBAK through ZBIRY, arranged alphabetically by name. Every subroutine name is also a link (keyword) for retrieving the corresponding description if you start at the index.

Also, online documentation (comment prologs) for individual user-callable SLATEC routines is available through the open-network LINMath (page 11) Web site.

PMATH Library

The PMATH mathematics subroutine library (libpmath.a) is a portable version of the CAL-coded part of the former MATHLIB library (libmath.a), with a few extra routines added, for a total of 68 routines. PMATH supplements but does not duplicate the SLATEC library.

LC's former Mathematical Software Services group developed portable versions of the CAL-coded part of MATHLIB. This machine-independent mathematics subroutine library they called PMATH (libpmath.a). While the original MATHLIB was only available on LC's CRAY Y-MP computers, PMATH is also available on LC's AIX (IBM) and Linux production computers (open and secure). Also, PMATH source code is available from the LINMath (page 11) Web site for you to download, move to, and compile on any future platform that you wish.

Documentation for PMATH originally consisted of its design specification, an inventory of routines, and 68 separate SLATEC-style explanatory prologs. Now all this material has been organized into the 135-page PMATH Library Reference Manual (URL: https://computing.llnl.gov/LCdocs/pmath), which is available online through LC's documentation servers (both open and secure). Early sections of this manual explain the design principles (including the name-choice principles) for the PMATH library and how they were implemented. Because of the close connection between MATHLIB and PMATH, the PMATH manual introduces the PMATH routines using their MATHLIB counterparts, and notes which MATHLIB routines were omitted from PMATH. A conversion chart between the MATHLIB and PMATH names is included. The PMATH rountines are also listed by functional group (statistical routines, ODE solvers, etc.) under their own names, with features of the newly added routines explained. The largest part of this manual by far is an alphabetical dictionary of PMATH routines and the descriptive prologs for each, including the calling sequence.

MSSL

MSSL (the Mathematical Software Service Library) is a collection of (Fortran) source code that is made available to LC users via the LINMath (page 11) Web site. (Source code distributed from LINMath can then be moved to other machines if you wish.)

From its inception, MSSL was divided into three parts:

MSSL1 (Class 1): fully-supported routines.
Online documentation available. This class includes many of the Fortran routines in MATHLIB, as well as the best software resulting from CCSE (now CASC) research.

MSSL2 (Class 2): minimally-supported routines.
No online documentation. These routines are generally good quality, but probably originated outside LLNL.

MSSL3 (Class 3): unsupported routines.
No online documentation except for code comments delivered by LINMath. (page 11) Use these at your own risk (but many of these 300 routines are high-quality software). Use the MSSL3 service routines (page 29) instead of those in SLATEC for more accurate results.

LC no longer distinguishes between Class 1 and Class 2. These two classes have been merged and are referred to collectively as simply MSSL (about 100 routines). Once you identify a relevant MSSL routine using the LINMath Web site help aids, you can (and must) retrieve any available documentation for it using LINMath as well. There is no separate MSSL reference manual. Online documentation is available for all user-callable MSSL routines via LINMath.

MATHLIB

The CRAY-based UNICOS library MATHLIB disappeared from LC along with the last Y-MP machine. See the PMATH (page 18) section above for information on the 68 MATHLIB routines whose portable versions are now provided through the PMATH library.

FFTW Library

FFTW is a free, nonproprietary C subroutine library for computing the Discrete Fourier Transform (DFT) in one or more dimensions, of both real and complex data, and of arbitrarily large input size. FFTW also efficiently handles multiple, strided transforms.

FFTW ("Fastest Fourier Transform in the West") was developed by Matteo Frigo and Steven G. Johnson at MIT. Version 2.1.5 (September, 2004) has been installed in these (double precision) files on LC's open (OCF only) AIX and Linux machines:

```
/usr/local/lib/libfftw.la
/usr/local/lib/libfftw.a
/usr/local/lib/librfftw.la
/usr/local/lib/librfftw.a
/usr/local/include/fftw.h
/usr/local/include/rfftw.h
```

A different version of FFTW (3.1.2) with an API that is incompatible with all 2.x versions of the library is separately available at

```
/usr/local/lib/libfftw3.a
```

FFTW is released under the GNU general public license. It works on any platform with a C compiler, and it is also callable from Fortran. Its authors claim that it has benchmarked to be "superior to other publicly available FFT software."

Of special interest to LC users is FFTW's support for parallelization. FFTW offers parallelized code for SMP machines with POSIX threads (URL: https://computing.llnl.gov/LCdocs/pthreads) (pthreads). And an MPI (URL: https://computing.llnl.gov/LCdocs/mpi) version for distributed memory transforms is available as well.

For general information on the FFTW math library and background papers on its technical features, consult

`http://www.fftw.org`

For detailed online documentation in HTML (including a subroutine index), consult

`http://www.fftw.org/doc`

SPRNG Library

SPRNG is the Scalable Parallel Random Number Generators library, callable from both C and Fortran codes. About half of all supercomputer cycles now go to stochastic ("Monte Carlo methods") calculations, and the SPRNG library was developed specifically to support ASC Monte Carlo computations under an ASC Level 3 grant to Florida State University (a project originally sited at the University of Illinois).

As a shared, standard library for scalable pseudorandom number generation, SPRNG aims to:

- Provide an almost infinite supply of parallel pseudorandom number streams with good statistical properties within and among the streams,
- Allow pseudorandom number streams to be reproduced for computational verification, independent of processor load and number of processors used,
- Support creation of new unique pseudorandom number streams on a parallel machine without using interprocessor communication,
- Support serial and parallel code portability across platforms, and
- Provide several different types of pseudorandom numbers, all in a scalable manner.

SPRNG 2.0 includes all types of pseudorandom number generators in a single library (seldom needed), while SPRNG 1.0 (installed on LC machines) supplies each random number generator in its own library for efficiency.

SPRNG is preinstalled for public use on all LC ASC IBM (AIX) computers as well as on open and secure Linux/CHAOS machines.

In /usr/local/lib the name of each SPRNG library file reflects the kind of random number generator that it provides:

```
libcmrg.a    Combined Multiple Recursive Generator
liblcg.a     Linear Congruential Generator with Prime Addend
             (48-bit and 64-bit versions)
liblfg.a     Additive Lagged Fibonacci Generator
libmlfg.a    Multiplicative Lagged Fibonacci Generator
```

In /usr/local/include are three necessary support files:

```
sprng_f.h     Fortran header file
sprng.h       C header file
interface.h
```

The SPRNG library can be used in both serial and parallel code. If you use MPI with SPRNG, be sure to:

- Call MPI_Init *before* your first call to any SPRNG function, and
- Call MPI_Finalize *after* your last SPRNG function call.

The SPRNG support Web site at
http://sprng.cs.fsu.edu
briefly describes the SPRNG project and also links to free, online (HTML) user documentation, including a brief Quick-Start Guide, a more thorough User Guide, and a complete Reference Manual that covers every SPRNG function. Specific technical questions about the library can also be sent directly to sprng@cs.fsu.edu.

MKL Library

MKL is Intel's threaded Math Kernel Library, a good source for BLAS and LAPACK routines in the Linux environment.

MKL is available *only* on LC machines with x86-based chips (i.e., Hera, Yana, and Zeus on the open network or Hopi, Juno, and Minos on the secure network). The relevant Linux system subdirectories are:

```
/usr/local/tools/mkl/lib/     (the library files)
                     /include  (the include files)
                     /doc      (vendor documentation)
```

The Linux environment variable OMP_NUM_THREADS controls the number of threads spawned by the MKL routines (by default, MKL sets the number of threads equal to the number of processors where you run).

NCAR Library

BACKGROUND.

NCAR is a long-tested graphics-oriented programming library with over two dozen Fortran and C tools for data display. NCAR routines draw contours, maps, vectors, streamlines, surfaces, histograms, X-Y plots, or even specific weather visualizations. LC provides NCAR version 5.0, which is much faster than earlier versions, directly on all OCF and SCF production machines. This includes the following machine/operating-system combinations:

```
IBM/AIX
IBM/Linux
Intel/Linux (the CHAOS clusters)
SGI/IRIX64
```

PREPARATION.

To use the NCAR library on LC machines, simple type

```
use ncar
```

Dotkit will set the following variables (as well as MANPATH and PATH) for you automatically:

```
NCARG_ROOT
NCARG_LIB
NCARG_BIN
NCARG_MAN
```

For additional details about setup if you prefer not to use Dotkit or if you wish to invoke version 4.4.0, see the LC Graphics Software Web page on NCAR at:

https://computing.llnl.gov/vis/ncar.shtml

SUPPORT.

For more information on the NCAR library from its provider, see the resources at this Web site:

http://ngwww.ucar.edu

Interactive Math Tools

Two commercial interactive math programs, Mathematica and MATLAB, are available on most LC production machines (but versions may vary by operating system).

Mathematica

Mathematica, first created in 1988, is used for symbolic computation and complex analysis, as well as 2D and 3D graphics, and programming. Mathematica creates fully customizable, publication-quality, cross-platform electronic and printed documents with professional mathematical typesetting quality and it also generates Web-ready documents.

AVAILABILITY:
Mathematica (version 5.0) is now available as a public file on all OCF and SCF production machines, regardless of operating system.

FONTS:
In April 2005, LC replaced the former OCF font server for Mathematica (called cola.llnl.gov) with a new font server (called fonts-lc.llnl.gov). Macintosh and PC users will (probably) need to reconfigure their local X-windows software to use fonts-lc.llnl.gov now (consult your local desktop staff for help). UNIX desktop users will need to run

```
xset fp+ tcp/fonts-lc.llnl.gov:7100
```

before they run Mathematica (below) to enable proper font service.

For more information, please type

```
news math_fonts
```

on any LC production system.

INTERFACES:
Mathematica offers a choice of two interfaces: a text interface and a GUI interface. No initialization file is needed to use Mathematica. To start the *text* interface, type

```
math
```

There are a limited number of licenses on each LC host. When you log into the program, if no license is available, you will receive a message indicating that the license limit has been reached or that no license was returned.

To use the GUI interface, log on using an X terminal or Xterm simulator and type

```
mathematica
```

Mathematica is located at /usr/local/bin/mathematica (which is really a link to /usr/global/tools).

SUPPORT:
To read more about Mathematica, consult Stephen Wolfram's *Mathematica, A System for Doing Mathematics by Computer*, which is considered the definitive source. There are also numerous Web sites available.

Two Web sites from the vendor are highly relevant:

http://www.wolfram.com/products/mathematica/introduction.html
(features introductory and tutorial background)
http://support.wolfram.com
(offers numerous support FAQs and help alternatives)

These additional nonvendor sites may also be of interest:

http://www.math.utep.edu/Mathematica/contents.html
http://smc.vnet.net/mathbench.html
http://smc.vnet.net/MathGroup.html
http://www.wri.com
http://www.mathematica-journal.com/home/

MATLAB

MATLAB is an interactive matrix "laboratory" developed and distributed by MathWorks. It is used for tasks involving matrices, graphics, and general numerical computation.

Starting in April 2003, MATLAB became available on LC's AIX (IBM) machines (but only 3 licenses on OCF, 8 licenses on SCF). If the licenses are being used, you will receive a warning telling you to "get a valid password." In summer 2004, MATLAB version 7 (and in January 2006, version 7.1) became available on all of LC's Linux (CHAOS) clusters. The MATLAB vendor also stopped supporting Tru64 and AIX, so local versions on LC's AIX IBM machines will remain frozen at level 6.5.

MATLAB is fairly straightforward to use. The underlying algorithms for MATLAB's built-in functions and supplied m-files are based on the standard libraries LINPACK and EISPACK. In addition, there are numerous extensions you can download from the Internet.

To run MATLAB, log on using an X terminal or Xterm simulator, and type

```
matlab
```

(or, to get version 7.1 on machines where that is not the default, use the pathname /usr/local/bin/matlab7.1). You can reach MATLAB's help documentation by typing helpwin at the prompt. A separate window opens and provides a list of help topics. Click the help topic you want to get more information. You can also type helpdesk or visit the MathWorks Web site.

Helpful Web sites include

http://www.glue.umd.edu/~nsw/ench250/primer.htm
http://www4.ncsu.edu/unity/users/p/pfackler/www/MPRIMER.htm
http://www.mathworks.com/products/matlab/

Tecplot

ROLE.

Tecplot is a commercial tool for interactive engineering plotting (X-Y, 2-D, and 3-D graphs) and for exploratory data visualization (contour plots, animation, etc.). The current version (Tecplot 360, successor to Tecplot 10) supports very large data sets and offers parallel processing.

AVAILABILITY.

Tecplot resides in the file /usr/global/tools/Tecplot on all LC production clusters, both AIX and Linux/CHAOS (Tecplot is not on BlueGene/L but it is supported on LC's special visualization machines). Tecplot requires "Open GL X Extension" (GLX) on your local workstation (X terminal) for proper display. One workaround is to invoke the Mesa graphics library instead, by using the -mesa option when you execute Tecplot.

USAGE.

To run Tecplot on LC machines, just type

```
tec360
```

(for the default version, no special environment-variable settings are needed).

SUPPORT.

For more background on how Tecplot works in the local environment, see its LC Graphics Software Web page for Tecplot at

`https://computing.llnl.gov/vis/tecplot.shtml`

For commercial documentation on Tecplot, see the vendor support page (again, OCF only) at

`http://www.tecplot.com/support/360/docs.aspx`

NVIDIA and Mesa Under Linux

Before CHAOS 3.2, the Mesa graphics library and the NVIDIA graphics library interfered with each other on LC Linux/CHAOS clusters (because the operating system allowed the NVIDIA installer to overwrite Mesa libGL files in /usr/lib64 or /usr/lib).

Starting with CHAOS 3.2 (spring 2007), NVIDIA files are installed in /usr/nvidia instead of /usr/lib64. The X-server configuration file and the system default library search path now look for libGL in /usr/nvidia *before* checking the usual library directories. And X11 now always renders with NVIDIA rather than with Mesa.

The chart below shows the default (mixed) graphics library and default include files on LC Linux clusters running CHAOS 3.2 or later versions. It also shows how you can switch to the alternative, nondefault library or include files if either default setting is not best for your work:

	Graphics Library	**Include Files**
Default	NVIDIA libGL	Mesa include files
Change GL to Mesa	Put /usr/lib64 into LD_LIBRARY_PATH environment variable	
Change includes to NVIDIA's		Compile with -I /usr/nvidia/include g++ option

Largest and Smallest Numbers

AVAILABLE NUMBERS:

The largest (and smallest) numbers that you can represent depend on the machine (chip set) that you are using, the compiler that you are using, and the data type (single precision, double precision, or integer). Follow these steps to discover the values most relevant to your needs:

(1) Select your

- target machine,
- target compiler (if several are available), and
- data type (single, double, integer).

(2) Log on to the target machine.

(3) Run any Web browser and supply the open or secure URL for LINMath, (page 11) LC's online math software source.

(a) On the LINMath home page, scroll down to the bottom, to the "GAMS Master Index."

(b) Select Category R (Service Routines).

(c) On the page that arrives next, select R1 (Machine-dependent constants).

(d) On the page that arrives next, select the MSSL3 library. WARNING: LINMath will also offer you routines in the SLATEC library, but avoid those. The SLATEC largest/smallest reporting routines have internal flaws that make them obsolete and unreliable on current LC machines.

(e) On the page that arrives next (MSSL3), select from these three routines those that meet your needs:

```
      R1MACH   for single precision,
   D1MACH   for double precision,
   I1MACH   for integer values.
```

When commented source code (Fortran, with a C version imbedded in the comments) for each routine displays, save it to a file by using your browser's FILE menu.

(4) On your target machine using your target compiler, compile and run a test code invoking the MSSL3 routine that reports current local information on the data type of interest to you, where

```
      R = R1MACH(1) reports the smallest positive magnitude,
   R = R1MACH(2) reports the largest positive magnitude,
   R = R1MACH(3) reports the smallest relative spacing,
   R = R1MACH(4) reports the largest relative spacing,
   R = R1MACH(5) reports the log10 of the arithmetic base
       (usually 2).

   D = D1MACH(1) through (5)
       reports same as R except double precision.

   I = I1MACH(9) reports the largest integer magnitude,
   I = I1MACH(12) reports the smallest exponent (single precision),
   I = I1MACH(13) reports the largest exponent (single precision),
   I = I1MACH(15) reports the smallest exponent (double precision),
   I = I1MACH(16) reports the largest exponent (double precision).
       [other integer values can be reported as well]
```

AVAILABLE PRECISION:

You may be more interested in the effect of various "precision" choices on how your calculations are carried out than on largest or smallest represented values per se. In that case, consult a subset of the OCF LC ASCI support Web pages to see the current local information on these precision topics:

- The *range* of binary, hexadecimal, character, and integer constants locally supported: https://computing.llnl.gov/code/content/fpe_source.php (URL: https://computing.llnl.gov/code/content/fpe_source.php)
- The allowed *byte sizes* for integer or real statements: https://computing.llnl.gov/code/content/fpe_statements.php (URL: https://computing.llnl.gov/code/content/fpe_statements.php)
- The specific *effects* of choosing double precision or double complex data types: https://computing.llnl.gov/code/content/fpe_double_options.php (URL: https://computing.llnl.gov/code/content/fpe_double_options.php)

Disclaimer

Keyword Index

To see an alphabetical list of keywords for this document, consult the next section (page 33).

Keyword	Description
entire	This entire document.
title	The name of this document.
scope	Topics covered in this document.
availability	Where these programs run.
who	Who to contact for assistance.
introduction	Role and goals of this document.
math-support-group	Former MSS group role.
math-chart	Chart of math libraries.
aix-libraries	Math libraries installed under AIX.
nmg	Numerical mathematics guide (retired).
linmath	Numerical math Web site (tool).
linmath-features	LINMath features summarized.
linmath-documentation	LINMath and GAMS manuals introduced.
linmath-packages	Math packages that LINMath supports.
math-libraries	Nonproprietary LC libraries.
slatec	SLATEC library overview.
slatec-background	History, role of SLATEC.
slatec-documentation	SLATEC manuals introduced.
pmath	PMATH library overview.
mssl	MSSL library overview.
mathlib	MATHLIB library (replaced/defunct).
fftw	FFTW library overview.
sprng	SPRNG library overview.
mkl	MKL library overview.
ncar	NCAR library overview.
math-tools	Commercial interactive math tools.
mathematica	Commercial symbolic math tool.
matlab	Commercial numerical math tool.
tecplot	Commercial plot and visualization tool.
nvidia	NVIDIA and Mesa interaction under Linux.
mesa	NVIDIA and Mesa interaction under Linux.
largest-numbers	Finding each machine's largest numbers.
smallest-numbers	Finding each machine's smallest numbers.
index	The structural index of keywords.
a	The alphabetical index of keywords.
date	The latest changes to this document.
revisions	The complete revision history.

Alphabetical List of Keywords

Keyword	Description
a	The alphabetical index of keywords.
aix-libraries	Math libraries installed under AIX.
availability	Where these programs run.
date	The latest changes to this document.
entire	This entire document.
fftw	FFTW library overview.
index	The structural index of keywords.
introduction	Role and goals of this document.
largest-numbers	Finding each machine's largest numbers.
linmath	Numerical math Web site (tool).
linmath-features	LINMath features summarized.
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math-chart	Chart of math libraries.
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mkl	MKL library overview.
mssl	MSSL library overview.
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pmath	PMATH library overview.
revisions	The complete revision history.
scope	Topics covered in this document.
slatec	SLATEC library overview.
slatec-background	History, role of SLATEC.
slatec-documentation	SLATEC manuals introduced.
smallest-numbers	Finding each machine's smallest numbers.
sprng	SPRNG library overview.
tecplot	Commercial plot and visualization tool.
title	The name of this document.
who	Who to contact for assistance.

Date and Revisions

Revision Date	Keyword Affected	Description of Change
07Jan09	entire	Remove references to retired machines; revise URLs where necessary.
	linmath	Revise URL of Web site.
	fftw	Remove old CHAOS, FFTW version numbers.
	mkl	Remove references to retired machines. Revised path to library files.
	slatec	SLATEC no longer installed or supported at LC.
03Jul07	nvidia	New section on NVIDIA/Mesa interaction.
	mesa	New section on NVIDIA/Mesa interaction.
	index	New keywords for new section.
	math-chart	Compaq/Tru64 column deleted.
	matlab	Compaq instructions deleted.
27Nov06	tecplot	New section introduces Tecplot 360.
	index	New keyword for new section.
11Oct06	aix-libraries	New section explains AIX math libraries.
	linmath-packages	New section lists downloadable packages.
	math-chart	Availability info expanded, updated.
	linmath-features	New URLs for LINMath sites.
	pmath	PMATH now installed under AIX.
	index	New keywords for new sections.
20Apr06	matlab	MATLAB version 7.1 now available.
	fftw	Relinking FFTW for use on CHAOS 3.
05May05	mathematica	New font server and support details.
12Jan05	ncar	New math/graphics library added.
	index	New keyword for new section.
	entire	TC2K retired, all sections.
28Sep04	linmath-documentation	GAMS print instructions updated.
	sprng	Blue deleted.
	matlab	MATLAB frozen on AIX, Tru64; version 7 now on OCF Linux clusters.
	fftw	Versions 2.1.5 and 3 separately available.
14Jan04	slatec	Former SLATEC_TOC deleted, unavailable.
17Jun03	mkl	Linux MKL library now available.
	index	New keyword for new section.
	math-chart	MASS (libmass.a) now on AIX.
	matlab	MATLAB now also on AIX.
03Dec02	availability	PMATH, SPRNG now on Linux.
	math-chart	PMATH, SPRNG now on Linux.
	pmath	Now on LC Linux machines.

	sprng	Now on LC Linux machines.
10Jun02	mssl	Better service routines noted.
	sprng	New math library added.
	largest-numbers	Finding largest, smallest numbers added.
	index	New keywords for new sections.
14Jan02	math-chart	Availability table revised.
	fftw	New math library added.
	linmath	LINMath has most recent sources.
	index	New keyword for new section.
20Mar01	math-tools	New section on interactive tools.
	index	New keywords for new section.
22Mar00	entire	CRAYs retired, all CRAY and NMG references suitably revised.
17Aug99	linmath	New URL, SCF version added.
	mathlib	Replaced by PMATH, details deleted.
	entire	All MATHLIB comments revised, keywords deleted.
23Jul98	linmath	LINMath Web site added, role noted throughout the text.
12Aug97	entire	First edition of this document.

EJG (07Jan09)